SRM Number: 1543 (Renewals)
MSDS Number: 1543
SRM Name: GC/MS System Performance Standard
Issued: March, 1992

MATERIAL SAFETY DATA SHEET

National Institute of Standards and Technology
Standard Reference Materials Program
Gaithersburg, Maryland 20899
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SECTION I. MATERIAL IDENTIFICATION

Material Name: GC/MS System Performance Standard

Description: SRM 1543 consists of four solutions; two concentrations of methyl stearate, and two concentrations of benzophenone in hexane.

Other Designations: Methyl Stearate (methyl octadecanoate) **and Benzophenone** (diphenylketone) **in Hexane** (n-hexane; hexyl hydride)

Chemical Formulas:

$CH_3(CH_2)_4CH_3$	(hexane)
$CH_3(CH_2)_{16}CO_2CH_3$	(methyl stearate)
$(C_6H_5)_2CO$	(benzophenone)

CAS Reg. Nos.:

110-54-3	(hexane)
112-61-8	(methyl stearate)
119-61-9	(benzophenone)

DOT Classification: Flammable Liquid
ID#: UN 1208

Manufacturer/ Supplier: Available from a number of suppliers.

SECTION II. HAZARDOUS INGREDIENTS

Hazardous Components	Nominal Concentration	Limits and Toxicity Data
Methyl Stearate	1.0 ng/ΦL (low) 5.0 ng/ΦL (high)	*N/A
Benzopnenone	1.0 ng/ΦL (low) 5.0 ng/ΦL (high)	*N/A
Hexane	Balance	**ACGIH TLV-TWA: 50 ppm /8 hrs or 180 mg/m^3 Human, Inhalation (CNS Effects): TC_{LO}: 5000 ppm/10 min Mouse, Inhalation: LC_{LO}: 120 gm/m^3

***T**hese materials are present in concentrations of less than 1.0% and do not require individual MSDS information under current OSHA regulations. For the actual concentrations of these compounds, refer to the corresponding Certificate of Analysis.

******ACGIH level set to prevent possible nerve cell damage.

SECTION III. PHYSICAL/ CHEMICAL CHARACTERISTICS

Hexane

Appearance and Odor: A clear, colorless, mobile fluid, with a mild hydrocarbon odor.
Molecular Weight: 86.18
Density: 0.65937*****
Boiling Point: ca 66 - 69 °C*****
Melting Point: -94.9 °C
Vapor Pressure (at 60 F): ca 100*****
Vapor Density (Air=1): 3
Volatiles (%): 100
Solubility in Water: Insoluble
Solubility in Other Compounds: Soluble in alcohol, acetone and ether.

*****Precise values depend on the grade of hexane.

SECTION IV. FIRE AND EXPLOSION HAZARD DATA

Flash Point (Hexane): -22.7 °C

(Method Used): closed cup

Autoignition Temperature: 260 °C

Flammability Limits in Air (Volume %): UPPER: ~ 7.5
LOWER: ~1.2

Extinguishing Media: Use carbon dioxide, dry chemical or foam. Water spray may be ineffective in putting out the fire and a water stream will spread the flames. A water spray, however, may be used to cool fire exposed cylinders to prevent pressure build-up and rupture.

Special Fire Procedures: Hexane is a highly flammable liquid (OSHA Class 1B flammable liquid). Firefighters should wear self-contained breathing apparatus along with proper eye and skin protection.

Unusual Fire and Explosion Hazards: When under pressure, this highly flammable substance is a dangerous fire hazard and a dangerous explosion hazard when heated. Vapor may travel over considerable distance to a source of ignition and flash back. Container explosion may occur under fire conditions. Fight fire from a safe distance; hexane burns like gasoline.

SECTION V. REACTIVITY DATA

Stability: __X__ **Stable** ____ **Unstable**

Conditions to Avoid: Keep this material from heat sources, sparks and open flames.

Incompatibility (Materials to Avoid): Keep this material from oxidizing agents.

See Section IV: Fire and Explosion Hazard Data.

Hazardous Decomposition or Byproducts: Thermal-oxidative decomposition products in air can include carbon monoxide.

Hazardous Polymerization: _____ **Will Occur** __X__ **Will Not Occur**

SECTION VI. HEALTH HAZARD DATA

Route of Entry: __X__ **Inhalation** __X__ **Skin** __X__ **Ingestion**

Health Hazards (Acute and Chronic): Excessive exposure to hexane vapors can cause upper respiratory tract irritation and CNS depression. In the body, n-hexane can be metabolized (partially oxidized) to a neurotoxin - *2,5-hexanedione*, which causes a nerve damage condition known as *peripheral polyneuropathy*, in individuals repeatedly exposed above 1000 ppm over a period of months.

Hexane is a defatting agent. Eye contact can be irritating; skin contact can cause irritation and *dermatitis* when it is repeated or prolonged. Ingestion may cause GI tract discomfort. Hexane acts as an aspiration hazard if vomiting occurs.

Signs and Symptoms of Exposure: Dizziness, numbness in the extremities, giddiness, and intoxication are symptomatic of hexane exposure depending on level and duration.

Medical Conditions Generally Aggravated by Exposure: N/A

Listed as a Carcinogen/Potential Carcinogen (Hexane):

	Yes	No
In the National Toxicology Program (NTP) Report on Carcinogens	____	X
In the International Agency for Research (IARC) Monographs	____	X
By the Occupational Safety and Health Administration (OSHA)	____	X

EMERGENCY AND FIRST AID PROCEDURES:

Skin Contact: Remove contaminated shoes and clothing. Rinse affected area with large amounts of water followed by washing the area with soap and water. Contact medical assistance if necessary.

Eye Contact: Immediately flush eyes, including under the eyelids, with copious amounts of water for at least 15 minutes. Contact medical assistance if necessary.

Inhalation: If inhaled, remove the victim to fresh air. If breathing is difficult, give oxygen; if victim is not breathing, give artificial respiration. Contact medical assistance if necessary.

Ingestion: If ingested, wash out mouth with water. **DO NOT** induce vomiting! Hexane is an aspiration hazard! If spontaneous vomiting occurs, lower head to knee level. Give several ounces of edible oil to drink. Contact medical assistance immediately!

TARGET ORGAN(S) OF ATTACK: Central nervous system, respiratory system, skin, GI tract, liver and kidneys.

SECTION VII. PRECAUTIONS FOR SAFE HANDLING AND USE

Steps to be taken in Case Material is Released or Spilled: Establish plans and provide training prior to any emergency situation. When spills occur, exclude workers from area except those assigned to clean-up. Clean-up personnel must have proper protection against inhalation of vapors or contact with the liquid. Provide maximum explosion-proof ventilation. Eliminate ignition sources. Flush hexane away from sensitive areas with a cold water spray. **Flush to the ground not to a sewer!** Small amounts of liquid, or absorbed liquid can be allowed to evaporate with good ventilation or in a hood or open area; large spills should be picked up in a safe and appropriate manner for disposal.

Waste Disposal: Burn material in a chemical incinerator equipted with an afterburner and scrubber but exert extra care in lighting as this material is highly flammable! Follow all Federal, state and local regulations.

Handling and Storage: Prevent skin contact by use of impermeable gloves, aprons, boots, lab coats, etc. Prevent eye contact by use of safety glasses, goggles, or face shield with goggles or glasses.

Note: Contact lenses pose a special problem; soft lenses may absorb irritants and all lenses concentrate them. **DO NOT** wear contact lenses in the lab.

Store in tightly closed containers in a cool, well ventilated area.away from oxidizing agents and sources of ignition and heat. Protect containers from physical damage. Use non-sparking tools. Use metal safety cans for handling small amounts. Storage and handling must be suitable for an OSHA Class 1B flammable liquid. **No smoking** in areas of storage or use. Avoid breathing vapors! Prevent contact with skin and eyes! Do not ingest.

Eyewash stations and safety showers should be readily available to areas of handling and use. Exposure monitoring and recordkeeping requirements which have been proposed by NIOSH for alkanes should be instituted.

SECTION VIII. SOURCE DATA/ OTHER COMMENTS

Sources: Genium Publishing Corporation, MSDS No. 397, August, 1983.
Hawley's Condensed Chemical Dictionary, 11th ed., 1987.
Handbook of Chemistry and Physics, 70th ed., 1989 - 1990.
The Merk Index, 11th ed., 1989.
Webster's Ninth New Collegiate Dictionary, 1990.

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Note: Physical and chemical data contained in this MSDS are provided for use in assessing the hazardous nature of the material. The MSDS was prepared carefully, using current references, however NIST does not certify the data on the MSDS. The certified values for this material are given only on the NIST Certificate of Analysis.